Impact on Sea Surface Salinity Retrieval of Multi-source Auxiliary Data within the SMOS mission

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***Abstract*—Aiming to provide Sea Surface Salinity (SSS) maps with a spatio-temporal averaged accuracy of 0.1 psu, the SMOS community is increasingly focusing on the determination of a robust inversion scheme to enable SSS retrieval from L-band brightness temperature data. In the framework of the *"Synergetic Aspects and Auxiliary Data Concepts for Sea Surface Salinity Measurements from Space"* project, efforts have been oriented towards a quantitative analysis of SSS retrieval once different auxiliary data are plugged into the minimization procedure, providing statistical distributions of the spatio-temporal averaged errors.**

I. INTRODUCTION

The ESA's Soil Moisture and Ocean Salinity (SMOS) Mission is based on the MIRAS instrument concept: an L-band two-dimensional synthetic aperture radiometer with multi-angular and dual/full-polarimetric imaging capabilities.
Development of a robust and suitable inversion procedure is a challenging key issue for SMOS community, since errors in the required auxiliary parameters, as sea surface temperature (SST) and wind speed (U_{10}), induce errors themselves in the retrieval procedure.

Within the *"Synergetic Aspects and Auxiliary Data Concepts for Sea Surface Salinity Measurements from Space"* project [1], efforts have been primarily devoted to the definition of suitable processing schemes for providing reliable auxiliary data, either for sea surface temperature or for wind speed/roughness [2], [3].

The subsequent activity concerned the analysis of SSS retrievals once the above mentioned different auxiliary data are plugged into the minimization procedure. The main goal was to stress the retrieved SSS variation induced by the different auxiliary data, providing the rms accuracy and bias associated to the error.

II. METHODOLOGY

Simulated daily brightness temperatures corresponding to January 2003 were provided by IFREMER. Retrieved Sea Surface Salinity variability with respect to different auxiliary parameters was then investigated under the following inversion methodology features:

- *Levenberg-Marquardt method*;

Minimization procedure performed by means of the *Levenberg-Marquardt* iterative numerical algorithm.

- *Multi-parameter retrieval*;

Either Sea Surface Salinity, or both SST and U_{10}, are tuned around some reference values to minimize the error.

- *Upper and lower boundaries*;

Physical-based boundaries selected, forcing the solution within the chosen ranges. Considered ranges were 25-40 *psu* with respect to salinity, 0-20 °C for SST and 0-20 m/s for wind speed.

- *Auxiliary data rms*;

A priori knowledge of the expected standard deviation of each auxiliary dataset used in the restricted and mixed configurations (hereafter detailed), to stress the solution once the accuracy of the plugged data is known.

- *Empirical linear fit to Hollinger's data*;

Hollinger's linear fit [4] for brightness temperature geophysical correction used in the inversion model.

- *Monte Carlo realizations*;

Ten Monte Carlo simulations of each scenario performed in order to derive the standard deviation (σ) associated to each retrieval and derive the optimum weights (1/σ) to perform the temporal averaging.

- *MIRAS operation mode: Full-pol or dual-pol;*

SSS retrieval performed either in full-pol mode using T_h and T_v or in dual-pol mode using the first Stokes parameter ($I=T_x+T_y=T_h+T_v$) to optimize the noise.
Before applying the minimization algorithm, IFREMER-simulated brightness temperatures were registered to the official *ISEA_4_H_9* grid within the considered Region Of Interest (ROI), a mid-Atlantic test zone of 10° width.
The whole month of simulated T_bs generated using the *SSA* (Small Slope Approximation) direct model was analyzed plugging different couples' combinations of auxiliary data, aiming to stress the impact on retrieved salinity of the different geophysical inputs, evaluating either difference with respect to SST or variation with U_{10}.
Auxiliary multi-source data at disposal were the following [5]:

- Blended *QuickSCAT/NCEP* (National Center for Environmental Predictions) wind,
- *ECMWF* (European Center for Medium-range Weather Forecast) wind, and
- *QuickSCAT* satellite wind

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14. ABSTRACT

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used as sea surface roughness information (considered as a sea-state primary descriptor);

- *CMS SAF/OSI* (Satellite Application Facility/Ocean and Sea Ice) SST, and
- *Reynolds SST,* besides the
- *WOA* (World Ocean Atlas) *98* climatologic SSS field.

A meaningful retrieval configuration was achieved in two subsequent steps.

First attempt for addressing a proper retrieval scheme consisted in processing simulated data sets considering a restricted version of the cost function; a reference value was provided within a term for each parameter weighted to the expected standard deviation.

Nevertheless, analysing results and following several hints hereafter detailed, a second approach was later identified. The following simulations were performed enlarging climatologic SSS *rms* accuracy value and then, adding a fake bias to confirm that restrictions in the cost function force the salinity retrieved values to have a mean equal to the reference value, and a standard deviation equal to the standard deviation associated to the reference value.

Subsequent simulations were conceived as a restricted-like (mixed) algorithm version, but letting SSS as a completely free parameter, without any additional constraints.

III. SALINITY RETRIEVAL: ONE OVERPASS

Being the climatologic SSS field furnished with a *rms* accuracy of nearly 0.2 *psu*, the first version restricted algorithm behaved in a way that hid the retrieved variation due to different auxiliary data.

In the second approach simulations have been performed for four different auxiliary data couples, the two instrument's operation modes (full-pol and dual-pol) and separated satellite passes (ascending and descending), resulting in sixteen monthly dataset to be processed. Yet, other simulations were carried out without considering any reference values, that is, no auxiliary parameters were plugged in the minimization procedure, which had to achieve convergence without any constraints.

Four different configurations were identified aiming at stressing firstly the variability with respect to auxiliary wind (blended wind, ECMWF and QuickScat) keeping constant SST, and secondly with respect to a different SST field (Reynolds), assuming reference blended wind.

As in the previous section, Fig. 1a shows error maps relevant to different configurations in dual-pol mode (i.e. using first Stokes parameter) for ascending pass corresponding to January 7th. The visibility of satellite tracks is clearly seen as well as the SSS error variability with respect to the different auxiliary data (hard to distinguish in the restricted configuration). Fig. 1b plots the number of times each pixel is imaged within the current day for the ascending pass.

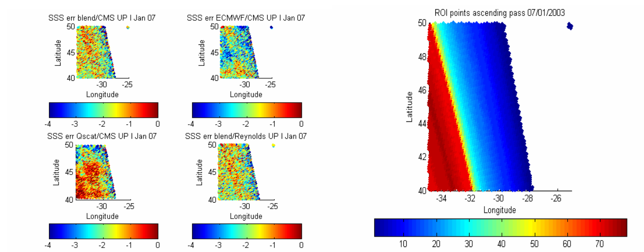

Fig. 1 a) Salinity single-overpass error maps for different configurations in dual-pol mode using I, and b) number of points used in the retrieval procedure. Both for ascending pass and corresponding to January 7th, 2003

IV. SALINITY RETRIEVAL: SPATIO-TEMPORAL AVERAGING

Towards the definition of the best SSS L2 product, spatio-temporal averaging has been approached as follows: Concerning temporal averaging, the above mentioned SSS errors have been averaged along the month but, providing the huge day-by-day variability of such SSS errors due to the different positions within the field of view (distance from the cross-track), a weighted mean was needed. Such weights are identified as the inverse of the standard deviations of the different realizations of each pixel, computed from the 10 Monte-Carlo realizations. Each single-pixel retrieval value was used to obtain weights for an adequate evaluation of the monthly error at pixel level. Pixels with retrieved SSS error farther away than $\pm 2.5\sigma_{sss}$ from the median (most probable value) are discarded as wrong. Afterwards, an overall ROI mean and rms furnished the expected bias and accuracy of each time-analysed configuration.

Fig. 2a shows the monthly geographical distribution of the weighted errors within the ROI for the blend/CMS (cfr. auxiliary data listed in the previous section) configuration in the ascending pass. Fig. 2b depicts the above values as histogram, underlying the monthly expected bias and the rms accuracy, the latter taken as retrieval goodness index in this study. This bias, being quite homogeneous in the whole ROI can be compensated for by means of an external calibration using e.g. moored buoys or drifters [6].

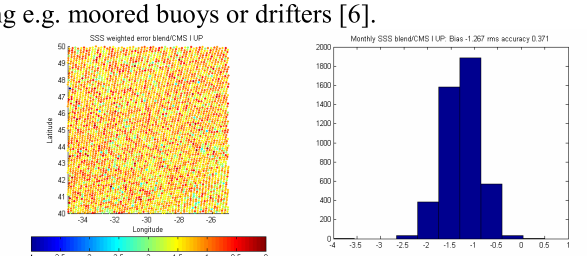

Fig. 2 a) Monthly ROI weighted errors relevant to blend/CMS configuration in dual-pol mode for the ascending pass. b) Monthly SSS weighted errors histogram with ROI bias and *rms* accuracy referred to blend/CMS configuration in dual-pol mode

As it can be seen in Table I, different configurations exhibit quite different values for the expected biases and rms accuracies. It has to be stressed, however, that the blend/CMS configuration represents the ideal case, being the auxiliary data used in brightness temperatures generation via the direct model, and all the retrievals obtained using other data combinations are supposed to be worse.
On the other hand, this novel mixed retrieval procedure succeeded in providing SSS variability due to different auxiliary parameters, which was the purpose of this study.
The following table summarizes the results gathered so far for each configuration

TABLE I. MONTHLY-AVERAGED BIAS AND RMS ACCURACY FOR THE DIFFERENT CONFIGURATIONS

Configuration	Pol. Mode	Satellite pass	Monthly Bias	rms accuracy
Blend/CMS	Dual (Stokes I)	UP	-1.267	0.371
Blend/CMS	Dual (Stokes I)	DN	-1.311	0.382
ECMWF/CMS	Dual (Stokes I)	UP	-1.361	0.491
ECMWF/CMS	Dual (Stokes I)	DN	-1.593	0.549
Qscat/CMS	Dual (Stokes I)	UP	-1.472	0.546
Qscat/CMS	Dual (Stokes I)	DN	-1.530	0.513
Blend/Reynolds	Dual (Stokes I)	UP	-1.258	0.368
Blend/Reynolds	Dual (Stokes I)	DN	-1.316	0.395
No aux data	Dual (Stokes I)	UP	-0.860	1.505
No aux data	Dual (Stokes I)	DN	-0.791	1.195
Blend/CMS	Full (Th/Tv)	UP	-1.447	0.337
Blend/CMS	Full (Th/Tv)	DN	-1.462	0.331
ECMWF/CMS	Full (Th/Tv)	UP	-1.512	0.401
ECMWF/CMS	Full (Th/Tv)	DN	-1.679	0.443
Qscat/CMS	Full (Th/Tv)	UP	-1.584	0.469
Qscat/CMS	Full (Th/Tv)	DN	-1.622	0.411
Blend/Reynolds	Full (Th/Tv)	UP	-1.443	0.346
Blend/Reynolds	Full (Th/Tv)	DN	-1.453	0.330
No aux data	Full (Th/Tv)	UP	-3.457	0.902
No aux data	Full (Th/Tv)	DN	-3.295	0.893

Several considerations arise from the results shown in the table:

- Concerning the auxiliary wind impact, ECMWF and QuickScat winds turned out to be worse than blended wind, with the second one mostly providing an even higher accuracy value.
- Concerning auxiliary SST impact, minimum effect is encountered supplying Reynolds field with the standard CMS one. One possible reason is that expected rms values plugged as reference in the algorithm for both fields are really close; besides, T_b sensitivity with respect to SST is quite low at 35 *psu*.
- Generally, descending passes provides a worse retrieval.
- Generally, the use of Th and Tv measured in full-pol mode provides a slightly better rms accuracy, but a slightly worse bias than using the first Stokes parameter measured as I=Th+Tv=Tx+Ty in dual-pol mode.
- Concerning unrestricted (no reference values) retrieval algorithm version, dual-pol mode provides a lower bias even if associated with a high accuracy value.

Regarding the latter consideration, a possible suggestion to correct for the remarkable bias encountered in the restricted configurations, might be performing retrieval firstly with an unrestricted configuration to allow bias correction, and then moving to restricted (with respect to SST and U_{10}) version to obtain better SSS retrieval accuracy performances.

Once the temporal averaging has been studied for different configurations, a spatial averaging is conducted in 1ºx1º and 2ºx2º boxes. Single-pixel weighted errors coming from temporal processing have been sorted regarding their geographic locations within the ROI and then averaged in the single boxes. Fig. 3a illustrates the 1ºx1º averaged values of the temporally-averaged SSS errors for blend/CMS configuration. Fig. 3b depicts the corresponding histogram and the relevant spatio-temporal bias and rms accuracy. As it can be appreciated bias is obviously the same, but the rms accuracy has decreased as expected, mostly according to the $\sqrt{N}$ factor; corresponding SSS accuracy turned out to be the best performance in the 1ºx1º spatial averaging scheme, achieving a remarkable value of 0.055 *psu* fulfilling the GODAE requirements [7]

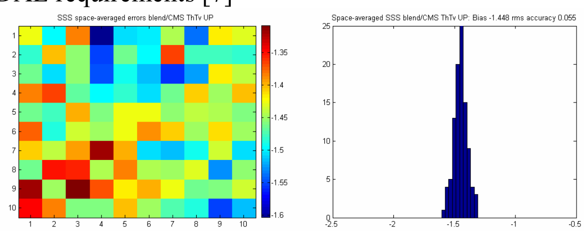

Fig. 3 a) ROI space-averaged (1ºx1º) SSS errors relevant to blend/CMS configuration in full-pol mode for the ascending pass. b) Space-averaged SSS histogram with spatio-temporal bias and *rms* accuracy referred to blend/CMS configuration in full-pol mode.

As with respect to temporal averaging, Table II summarizes spatio-temporal SSS rms accuracy for each configuration, polarimetric mode and satellite pass:

TABLE II. SPATIO-TEMPORAL RETRIEVED SSS RMS ACCURACY FOR THE DIFFERENT CONFIGURATIONS. IN RED: SMALLEST SSS ERROR. IN GREEN: CONFIGURATIONS SATISFYING GODAE REQUIREMENTS.

Configuration	Pol. Mode	pass	*rms* 1ºx1º	*rms* 2ºx2º
Blend/CMS	Dual (Stokes I)	UP	0.071	0.050
Blend/CMS	Dual (Stokes I)	DN	0.099	0.080
ECMWF/CMS	Dual (Stokes I)	UP	0.264	0.248
ECMWF/CMS	Dual (Stokes I)	DN	0.293	0.273
Qscat/CMS	Dual (Stokes I)	UP	0.309	0.291
Qscat/CMS	Dual (Stokes I)	DN	0.206	0.162
Blend/Reynolds	Dual (Stokes I)	UP	0.078	0.057
Blend/Reynolds	Dual (Stokes I)	DN	0.102	0.081
No aux data	Dual (Stokes I)	UP	0.835	0.737
No aux data	Dual (Stokes I)	DN	0.431	0.326
Blend/CMS	Full (Th/Tv)	UP	0.055	0.036
Blend/CMS	Full (Th/Tv)	DN	0.061	0.032
ECMWF/CMS	Full (Th/Tv)	UP	0.186	0.166
ECMWF/CMS	Full (Th/Tv)	DN	0.212	0.198
Qscat/CMS	Full (Th/Tv)	UP	0.234	0.220
Qscat/CMS	Full (Th/Tv)	DN	0.136	0.097
Blend/Reynolds	Full (Th/Tv)	UP	0.070	0.045
Blend/Reynolds	Full (Th/Tv)	DN	0.056	0.035
No aux data	Full (Th/Tv)	UP	0.289	0.207
No aux data	Full (Th/Tv)	DN	0.259	0.211

V. CONCLUSIONS

In this SSS retrieved study, the following assumptions have been made:
- Perfect Faraday rotation and atmospheric corrections,
- Perfect sea water dielectric constant model, but
- Different brightness temperature dependence with wind speed in the direct and inverse models (SSA model vs. linear fit to Hollinger's data).

Under the above assumptions the use of Th and Tv measured in full-pol mode provides a slightly better rms SSS error by a 1.1-1.2 factor, but a slightly worse bias than using the first Stokes parameter measured as I=Th+Tv=Tx+Ty in dual-pol mode.

Being aware that possible sources of discrepancies lie in the fact that simulated brightness temperatures were generated without bias and that models used in the direct and inverse procedure were different (SSA model vs. linear fit to Hollinger's data), major conclusions are the following:

One overpass SSS retrieval:
- SSS error in absolute value is mostly around 1 *psu* (varying depending on the auxiliary data plugged) increasing up to 4 *psu* or more at swath edges, in agreement with [8], [9] and [10].
- A bias appears in the measurements and must be corrected for by using ground-truth data (e.g. buoys or drifters).

Temporal averaging of retrieved SSS:
- Performed as the weighted mean of the retrieved SSS by the inverse of the standard deviation.
- 30-day temporal averaging at pixel level has an rms error within the range 0.33-0.55 psu, depending on the auxiliary dataset used.
- As expected best results are obtained for the auxiliary data set with which the original brightness temperatures were generated: Blend U_{10} and CMS SST. Worse results are obtained for QuickScat and ECMWF wind data.
- The use of different sources of auxiliary data for SST has a minimum impact in the SSS retrieval.
- Usually, the descending pass provides a worse SSS retrieval than ascending pass.
- Averaging ascending and descending passes does not decrease the error by a $\sqrt{2}$ factor, since they exhibit different biases (Table I).

Spatiotemporal averaging of retrieved SSS:
- In a period of 30 days and 1ºx1º boxes the retrieved rms SSS error ranges between 0.055 - 0.3 psu.
- In a period of 30 days and 2ºx2º boxes the retrieved rms SSS accuracy ranges between 0.032 - 0.29 psu
- The **best SSS products** obtained by spatiotemporal averaging of **30 days,** both largely **within the GODAE requirements**]. are**:**
- Concerning **1ºx1º boxes: ascending overpasses**, using **blended wind data**, and **CMS SAF/OSI SST data** with a rms error of 0.055 psu;
- Concerning **2ºx2º boxes: descending overpasses**, using **blended wind data**, and **CMS SAF/OSI SST data** with a rms error of 0.032 psu.

This result has to be taken with caution, since the original brightness temperature data were generated with the same wind field.
For example, if ECMWF data are used instead, the rms error increases up to 0.2-0.3 psu (depending on instrument's configuration and satellite pass). Other studies [6], [11] have shown that without auxiliary data and after spatio-temporal averaging (30 days, 1ºx1º), SSS rms error ranges from 0.2 psu at the Equator to 0.7 psu in Polar regions.

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